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Projection technique and Bloch functions

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In the present article, the use of projection technique as a tool for investigating properties of Bloch functions, is demonstrated. Having first established the necessary prerequisities, a general form for the projection operators relevant to cyclic operators, is derived. This form is then used to construct the projection operators for translation operators relevant to crystal lattices. With the help of these projection operators, it is shown finally that any arbitrary function satisfying Born-Von Karman boundary condition, is resolvable into components which are identical to Bloch functions. The treatment is given with reference to a N-dimensional lattice, the results for the ordinary three dimensional case being obtainable by putting $N = 3$

1. Introduction

The idea of projection operators, introduced first by non Neumann (Von Neumann 1955), is of great utility for various quantum mechanical studies In particular, the concept has been used ubiquitously for investigation of atomic and molecular systems within the framework of Hartree-Fock theories (Huzinaga *et al* 1973, Roothan 1960; Silverstone & Yin 1968)

In the present article, we show how the technique of projection can be used to elucidate the properties and role of Bloch Functions which characterise, as is well known, the motion of electrons in crystalline solids Having introduced some fundamental definition and derived certain features therefrom, we establish the product form of projection operators and relevant generalisations. We then use these results to construct the projection operators associated with cylic operators whence, we obtain the projection operators for translation operators relevant to crystals. We finally use this last variety of projection operators to establish that, any arbitrary function satisfying the Born- Von Karman boundary condition is resolvable into components which possess all the properties of Bloch Functions. We have put, at the end, a comprehensive discussion about our findings.

In order to arrive at results of general nature, we have considered a N-dimensional lattice; the case of ordinary three dimensional lattice follows straightway with $N = 3$.

2. Basic Definitions and Related Features

In this section, we first introduce the definition of a projection operator and derive therefrom some results of general character.

A projection operator O_k is defined through the following operation

$$O_k\psi = a_k\psi_k = \phi_k \text{ (say)} \quad \dots \quad (1)$$

where,

$$\psi = \sum_{k=1}^{n} \phi_k \quad \dots \quad (2)$$

The relation (2) describes an expansion of ψ in terms of the set of functions ψ_k's and the relation (1) shows that O_k maps the function ψ onto its k-th component $\phi_k (= a_k\psi_k)$ or it selects the k-th component of the expansion for ψ.

With the help of eqs (1) and (2), we can derive easily the following results

(a) *O_k's are idempocent.* Since the repeated use of O_k means the selection of the k-th component out of k-th component, we have

$$O_k^2 = O_k \quad \dots \quad (3a)$$

$$O_k\phi_k = \phi_k \quad \dots \quad (3b)$$

The property (3a) is expressed by saying that O_k is idempotent and the same property earns, as a geometrical analogy, the name projection operator for O_k

(b) *O_k's are mutually exclusive* The selection of the k-th component out of the l-th component, necessarily gives a zero element. Thus,

$$O_kO_l = 0, \qquad \text{for } k \neq l, \quad \dots \quad (4a)$$

$$O_k\phi_l = 0, \qquad \text{for } k \neq l, \quad \dots \quad (4b)$$

The property (4a) is expressed by saying that O_k and O_l are mutually exclusive.

(c) *Resolution of identity.* In view of eqs (1) and (2), we have

$$\psi = \sum_k a_k\psi_k = \sum_k \phi_k$$

or

$$(I - \sum_k O_k)\psi = 0 \quad \dots \quad (5)$$

where I is the identity operator Eq. (5) is true for any arbitrary function Hence we must have

$$\sum_k O_k = I. \quad \dots \quad (6)$$

The relation (6) affords what we may call the *Resolution of identity* in terms of the projection operators O_k's.

(d) *Eigenprojectors.* So far, we have presented our discussion with reference to the expansion of an arbitrary function ψ in terms of the basis $(\psi_1, \dots, \psi_n)$, without any introduction of the operators, of which ψ_k's might be the eigenfunctions. We now suppose that ψ_k's constitute the spectrum of eigenfunctions of an operator A, the relevant eigenvalues being λ_k's, and establish an important connection between A and O_k's

Since ψ_k's are eigenfunctions to A with eigenvalues λ_k's, ϕ_k's are also eigenfunctions to A with the same eigenvalues. Hence, we may write

$$A\phi_k = \lambda_k\phi_k = \lambda_k(O_k\psi) = (\lambda_k O_k)\psi$$

or

$$(AO_k - \lambda_k O_k)\psi = 0. \qquad \ldots (7)$$

Since eq (7) is true for any arbitrary function ψ, we have

$$AO_k = \lambda_k O_k. \qquad \ldots (8)$$

The relation (8) above is the fundamental eigenvalue relation and O_k's may be characterised as eigenprojectors to A, with eigenvalues λ_k's

3. Product form of Projection Operators and Relevant Generalisation

In the previous section, we have established, via eq. (8), a link of O_k's with the operator A, of which ϕ_k's are eigenfunctions We now intend to obtain a form of O_k explicitly in terms of A and the eigenvalues λ_k This explicit form, known commonly as product form for its structure, is considerably useful for the study of many realistic problems.

Derivation of the product form To begin with, let us consider the product

$$\prod_{j\neq k} (A-\lambda_j I)\phi_l.$$

Since ϕ_l is an eigenfunction to A with eigenvalue λ_l, we have

$$\prod_{j\neq k} \{(A-\lambda_j I)\}\phi_l = \prod_{j\neq k} (\lambda_l-\lambda_j)\phi_l$$

$$= 0, \quad \text{for } l \neq k, \qquad \ldots (9)$$

$$= \prod_{k\neq j} (\lambda_k-\lambda_j)\phi_k, \quad \text{for } l \neq k, \qquad \ldots (10)$$

or,

$$\prod_{j\neq k} \left\{\frac{(A-\lambda_j I)}{(\lambda_k-\lambda_j)}\right\} \phi_l = \delta_{kl}\phi_k \qquad \ldots (11)$$

The relation (11) shows that the product $\left[\prod_{j\neq k} \frac{(A-\lambda_j I)}{(\lambda_k-\lambda_j)}\right]$ possesses the properties (3b) and (4b), characteristic of the projection operator O_k We have shown in the appendix that this product satisfies also the properties (3a), (4a), (6) and (8) Hence we can take it to be a form of the projection operator O_k

$$O_k = \prod_{j \neq k} \frac{(A-\lambda_j I)}{(\lambda_k-\lambda_j)}. \quad \dots (12)$$

Projection operators related to a set of commuting operators The Quantum-Mechanical investigation of many physical systems requires us to deal with a set of commuting operators The translation operators treated later provide an example of this kind of situations. We intend to discuss here certain features of the projection operators related to a set of commuting operators; the features thus derived would be used in subsequent analysis At first, we consider the case of two commuting operators and generalise the results later

Now, let A and B be two commuting operators with eigenvalues λ_k's and μ_l's In view of eq. (12), we can write

$$O_k(A) = \prod_{j \neq k} \left\{ \frac{(A-\lambda_j)}{(\lambda_k-\lambda_j)} \right\} \quad \dots (13)$$

$$O_l(B) = \prod_{i \neq l} \left(\frac{B-\mu_i}{(\mu_l-\mu_i)} \right). \quad \dots (14)$$

Since A and B commute, they have simultaneous eigenfulctions. If ϕ_{kl} is simultaneously an eigenfunction to A and B with eigenvalues λ_k and μ_l respectively, we have

$$A\phi_{kl} = \lambda_k\phi_{kl} \quad \dots (15)$$

$$B\phi_{kl} = \mu_l\phi_{kl} \quad \dots (16)$$

Further, in view of eq. (6), we have

$$I = [\sum_k O_k(A)][\sum_l O_l(B)] = \sum_{kl} O_{kl} \quad \dots (17)$$

where,

$$O_{kl} = O_k(A)O_l(B) \quad \dots (18)$$

It is now easy to derive the following results

$$O_{kl}^2 = O_{kl} \quad \dots (19)$$

$$(O_{kl})(O_{k'l'}) = 0; \quad \text{for } k = k',\ l \neq l'; \quad \dots (20)$$

$$AO_{kl} = \lambda_k O_{kl} \quad \dots (21)$$

$$BO_{kl} = \mu_k O_{kl} \quad \dots (22)$$

$$AB(O_{kl}) = \lambda_k\mu_l(O_{kl}). \quad \dots (23)$$

All the above results can be straightforwardly generalised to a set of more than two commuting operators A, B, C, ... etc. We record here the following cases which will be particularly used later

$$I = [\sum_{k,l,m\ldots} O_{klm\ldots}] = [\sum_{k,l,m\ldots} O_k(A)O_l(B)O_m(C)\ldots] \qquad \ldots \quad (24)$$

$$A[O_{klm\ldots}] = \lambda_k[O_{klm\ldots}] \qquad \ldots \quad (25)$$

$$[ABC\ldots][O_{klm\ldots}] = [\lambda_k\mu_l\nu_m\ldots][O_{klm\ldots}] \qquad \ldots \quad (26)$$

4. Projection Operators Relevant to Cyclic Operators

In this section, we derive the explicit form of projection operators related to *cyclic operators*, which we quite often come across in practice

An operator A is said to be cyclic of order G when it satisfies the condition

$$A^G = I. \qquad \ldots \quad (27)$$

If λ is an eigenvalue of A belonging to the eigenfunction ϕ, we have, in view of eq. (27),

$$A^G\phi = \lambda^G\phi = \phi$$

or,

$$\lambda^G = 1. \qquad \ldots \quad (28)$$

Relation (28) gives the spectrum of eigenvalues of λ_k's (totalling G) of A as

$$\lambda_k = \exp(2\pi i k/G) \qquad \ldots \quad (29)$$

where, $k = 0, 1, \ldots, (G-1)$.

With the help of eq. (29), we can write

$$\prod_{j=0}^{(G-1)} (A-\lambda_j) = F(A) \text{ (say)} = A^G-1. \qquad \ldots \quad (30)$$

Using eqs. (12) and (30) together and carrying out some simplifications we have the following form of the projection operator $O_k(A)$ relevant to a cyclic operator of order G

$$O_k(A) = \frac{1}{G}\sum_{l=0}^{(G-1)} \lambda_k^{-l}A^l \qquad \ldots \quad (31)$$

In view of the property (8), we have

$$AO_k(A) = \exp(2\pi ik/G)O_k(A) \qquad \ldots \quad (32)$$

5. Projection Operators Related to Translation Operators and Bloch Function in a N-Dimensional Lattice

So far, we have discussed certain aspects of projection operators in general. We now intend to construct the projection operators for the so-called translation operators related to the translational symmetry of crystals and examine the effect of their operation on arbitrary functions satisfying Born-Von Karman (BV) boundary condition; as we will see subsequently, this study reveals an important role of Bloch Functions.

Considering a N-dimensional lattice, we recollect that the translation operators T_i's are given by

$$T_i\phi(r) = \phi(r+a_i); \quad i = 1, 2 \ldots N, \qquad \ldots (33a)$$

$a_1, a_2, \ldots a_N$, are the N primitive translation vectors of the lattice. It is obvious from (33a) that T_i's commute with each other

$$T_iT_j = T_jT_i. \qquad \ldots (33b)$$

The lattice vectors, denoted by d are given by

$$\boldsymbol{d} = \sum_{i=1}^{N} d_i \boldsymbol{a}_i \qquad \ldots (34)$$

where, d_i's are positive or negative integers.

Putting, $\prod\limits_{i=1}^{N} T_i^{d_i} = T(d)$, we obviously have

$$T(d)\phi(r) = \phi(r+d) \qquad \ldots (35)$$

The reciprocal lattice is described, in the usual manner, by the primitive translation vectors, b_i's, given by

$$a_i\, b_j = \delta_{ij} \qquad \ldots (36)$$

The relations (33) to (35) provide all the basic characteristics of translation operators related to crystal lattices. Any further feature of T_i's would depend on specific characteristics of the functions $\phi(r)$ on which T_i's operate. Let us assume that $\phi(r)$ satisfies the 'BV' boundary condition

$$\phi(\boldsymbol{r}+G_i\boldsymbol{a}_i) = \phi(r); \quad i = 1, 2, \ldots N; \qquad \ldots (37)$$

where, G_ia_i = dimension of the lattice along a_i. Combining eqs (33) and (37), we have

$$T_i^{G_i} = I. \qquad \ldots (38)$$

Thus, when $\phi(r)$ satisfies 'BV' boundary condition, each of T_i's is a cyclic operato of order G_i. The projection operators corresponding to various T_i's are consequently given by eq (31). Explicitly, we have

$$O_{k_j}(T_j) = \frac{1}{G_j} \sum_{d_j=0}^{(G_j-1)} [\exp(-2\pi i k_j d_j/G_j)T_j^{d_j}] \qquad \ldots (39)$$

k_j is any of the integers : $0, 1, \ldots (G_j-1)$; with $j = 1, 2, \ldots N$

Further, we have

$$\prod_{j=1}^{N} O_{kj}(T_j) = \prod_{j=1}^{N} \frac{1}{G_j} \sum_{d_j=0}^{(G_j-1)} [\exp(-2\pi i k_j d_j/G_j) T_j^{d_j}]$$

$$= \frac{1}{G_1 \ldots G_N} \sum_{d_1 d_2 \ldots d_N=0}^{(G-1),\ldots(G_N-1)} \left[\exp\left\{-2\pi i\left(\sum_{j=1}^{N} k_j d_j/G_j\right)\right\} \prod_{j=1}^{N} T_j^{d_j}\right] \ldots \quad (40)$$

Let now k be a vector in the reciprocal lattice defined as

$$\boldsymbol{k} = \sum_{j=1}^{N} \frac{k_j b_j}{G_j}$$

Taking account of eq. (36) and the above vector k, we can bring eq. (40) to the following form

$$\prod_{j=1}^{N} O_{kj}(T_j) = \frac{1}{G_1 \ldots G_N} \sum_{d_1, d_2 \ldots d_N=0}^{(G_1-1),\ldots(G_N-1)} [\exp(-2\pi i k.d) T(d)]. \quad \ldots \quad (41)$$

Since T_i's form a set of N commuting operators, all results derived earlier for a set of commuting operators, are applicable to them. Making use of eq. (26), we get

$$T(d) \prod_{j=1}^{N} O_{k_j}(T_j) = \exp(ik.d) \prod_{j=1}^{N} O_{kj}(T_j). \quad \ldots \quad (42)$$

Also, in view of eq. (24), we have

$$\phi(r) = \sum^{(G_1-1),\ldots(G_N-1)} \{O_{k_1}(T_1) \ldots O_{kN}(T_N)\}\phi(r)$$

$$= \sum_{k_1, k \ldots k_N=0}^{(G_1-1),\ldots(G_N-1)} \phi_{k_1 \ldots kN,}(r) \quad \ldots \quad (43)$$

where,

$$\phi_{k_1 \ldots k_N}(r) = \{O_{k_1}(T_1) \ldots O_{kN}(T_N)\}\phi(r) \quad \ldots \quad (44)$$

From eq. (43), we see that any arbitrary function $\phi(r)$ satisfying BV boundary condition in a N-dimensional lattice, can be resolved into component $\phi_{k_1 \ldots k_N}(r)$; the total number G of such components is given by

$$G = (G_1 G_2 \ldots G_N). \quad \ldots \quad (45)$$

Let us now examine the properties of $\phi_{k_1 \ldots k_N}(r)$. With the help of eqs. (42) and (44), we have

$$T(d)\phi_{k_1 \ldots k_N}(r) = (\exp ik.d)\phi_{k_1 \ldots k_N}(r) \qquad \ldots \quad (46)$$

Combining eqs. (35) and (46), we further have

$$\phi_{k_1 \ldots k_N}(r+d) = (\exp ik.d)\phi_{k_1 \ldots k_N}(r) \qquad \ldots \quad (47)$$

Relation (46) shows that $\phi_{k_1 \ldots k_N}(r)$ is an eigenfunction to the translation operator $T(d)$, with the uni-modular complex quantity $(\exp ik.d)$ as its eigenvalue, while eq. (47) shows that $\phi_{k_1 \ldots k_N}(r)$ is connected to $\phi_{k_1 \ldots k_N}(r+d)$ through the multiplying factor $[\exp(ik.d)]$, these two properties of $\phi_{k_1 \ldots k_N}(r)$ are just the features which characterise completely the well known Bloch Functions. Hence, we establish that the members $\phi_{k_1 \ldots k_N}(r)$ of the set of functions, which forms the basis for the expansion of any arbitrary function $\phi(r)$ satisfying BV boundary conditions, are identical to Bloch Functions

6 Discussion

As mentioned in the introduction, the aim of this article is to elucidate how one can study a role of Bloch Functions with the help of projection operators relevant to translation operators In the previous section we have established that the Bloch Functions constitute the members of a set of functions, in terms of which, one can have an expansion of any arbitrary function $\phi(r)$ satisfying periodic (BV) boundary condition That the components serving as a basis of expansion for the afore-mentioned function $\phi(r)$, are indeed Bloch Function, has been established in a general way, with the help of projection formalism associated with translation operators (Relations (46) and (47)). It has also been shown that the total number of such Bloch components, necessary for the expansion of $\phi(r)$, is just equal to the total number of quantum states in any allowed band of energies (Relation (45)); this fact is often required for Quantum Mechanical investigation of crystalline solids. The properties of Bloch Functions as well as the role of Bloch Functions in the study of crystal physics, were examined (Bloch 1928) from the stand point of scular theory and later with the help of Group theory (Slater 1965). We demonstrate here that the projection technique affords another tool for a rigorous derivation of the characteristics of Bloch Functions.

Appendix

We furnish here the proofs regarding the validity of the properties (3a), (4a), (6) and (8), with respect to the product form of projection operators (From (12)).

The starting point for the desired proofs is the well known Caley-Hamilton theorem. This theorem reads as

$$P(A)=\prod_{j=1}^{n}(A-\lambda_j)=0 \qquad \ldots \text{ (I)}$$

where, A is an operator having the eigenvalues λ_k's (assumed non-degenerate) with the help of eqs (1) and (12), we have

$$(A-\lambda_k I)O_k=\frac{P(A)}{\prod_{j\neq k}(\lambda_k-\lambda_j)}=0 \qquad \ldots \text{ (II)}$$

or,

$$AO_k=\lambda_k O_k \qquad \ldots \text{ (III)}$$

(III) proves the condition (8).

The form (12) for O_k can be written as

$$O_k=\prod_{j\neq k}\left[\frac{(A-\lambda_k I)}{(\lambda_k-\lambda_j)}+I\right] \qquad \ldots \text{ (IV)}$$

Combining (II) and (IV), we have

$$O_k^2=O_kO_k=\left\{\prod_{j\neq k}\left[\frac{A-\lambda_k I}{\lambda_k-\lambda_j}+I\right]\right\}O_k$$

$$=O_k, \qquad \ldots \text{ (V)}$$

(V) shows that O_k's, given by eq (12) are idempotent i.e. they staisfy the property (3a).

Let us now consider the product O_kO_1, with O_k's given by eq (12) We have

$$O_kO_l=\left\{\prod_{j\neq k}\left(\frac{A-\lambda_j I}{\lambda_k-\lambda_j}\right)\right\}O_l$$

$$=\left\{\prod_{j\neq k,\, l}\left(\frac{A-\lambda_j I}{\lambda_k-\lambda_j}\right)\right\}\left(\frac{A-\lambda_l I}{\lambda_k-\lambda_l}\right)O_l$$

$$=0, \text{ in view of (II)}, \qquad \ldots \text{ (VI)}$$

(VI) proves the property (4a) regarding the mutual exclusiveness of O_k's

To prove finally the property (6) regarding the resolution of identity, we notice that for any complex variable z, we can write

$$O_k(z) = \prod_{j \neq k} \left(\frac{z-\lambda_j}{\lambda_k-\lambda_j} \right)$$

$$= \frac{P(z)}{(z-\lambda_k) \prod_{j \neq k} (\lambda_k-\lambda_j)}, \qquad \ldots \quad \text{(VII)}$$

From (VII), we see that $O_k(z)$ is a polynomial of degree $(n-1)$, having the value 1 for $z = \lambda_k$, and the value 0 for $j \neq k$. Let us now consider the function $G(z)$ given by

$$G(z) = 1 - \sum_{k=1}^{n} O_k(z) \qquad \ldots \quad \text{(VIII)}$$

Considering (VII) and (VIII) together, we see that $G(z)$ is a polynomial of degree $(n-1)$, having the value zero in the n-points

$$z = \lambda_1, \lambda_2, \ldots, \lambda_n.$$

$$G(z) = 0 \qquad \ldots \quad \text{(IX)}$$

The identity (IX) remains valid even if we replace the variable z by the operator A and the number 1 by the identity operator I. Thus we hace

$$I = \sum_{k=1}^{n} O_k(A). \qquad \ldots \quad \text{(X)}$$

The relation (X) proves the fundamental property (6).

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